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An interpolation algorithm for orthogonal rational functions

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Abstract

Let $A=\{\alpha_1,\alpha_2,\ldots\}$ be a sequence of numbers on the extended real line $\hat{\mathbb{R}}=\mathbb{R}\cup\{\infty\}$ and μ a positive bounded Borel measure with support in (a subset of) $\hat{\mathbb{R}}$. We introduce rational functions ϕ_n with poles $\{\alpha_1,\ldots,\alpha_n\}$ that are orthogonal with respect to μ (if all poles are at infinity, we recover the polynomial situation). It is well known that under certain conditions on the location of the poles, the system $\{\phi_n\}$ is regular such that the orthogonal functions satisfy a three-term recurrence relation similar to the one for orthogonal polynomials.

To compute the recurrence coefficients one can use explicit formulas involving inner products. We present a theoretical alternative to these explicit formulas that uses certain interpolation properties of the Riesz–Herglotz–Nevanlinna transform Ω_μ of the measure μ. Error bounds are derived and some examples serve as illustration.

MSC: 42C05; 65D05

Keywords: Orthogonal rational functions; Orthogonal polynomials; Three-term recurrence; Interpolation

1. Introduction

The theory of orthogonal rational functions has been widely studied over the last few decades, see e.g., the comprehensive monograph [1]. A possible approach to the subject is to consider orthogonal rational functions as generalisations of orthogonal polynomials or equivalently, orthogonal polynomials form a special case of orthogonal rational functions (with all poles fixed at infinity). Many classical results from orthogonal polynomials, such as those concerning recurrence relations, quadrature formulas, Favard theorems, moment problems, Padé approximation, etc. have been generalised to the case of orthogonal rational functions.

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However, much like the polynomial case (see e.g., Gautschi's comments in [5]), surprisingly little attention has gone to numerical and computational aspects, i.e., the question of constructing (computing) a set of rational functions given a certain orthogonality measure. In the polynomial case, most practical applications require the use of classical polynomials such as the Legendre or Chebychev polynomials, for which the recurrence coefficients are explicitly known. Maybe this accounts for the lack of interest in computational aspects. For the orthogonal rational functions however, we do not have such 'classical' cases (yet), which makes it all the more necessary to pay special attention to the actual construction of these functions.

In this paper it is our aim to present an interpolation algorithm to (theoretically) compute the recursion coefficients. A detailed error analysis will show, however, that this algorithm is of little practical use. In most cases the error will become unbounded. The algorithm gives rise to a continued fraction whose approximants are multipoint Padé approximants to the Stieltjes transform of the orthogonality measure, as discussed in [2]. In [4] we will present a more useful algorithm to compute the recurrence coefficients (at least for the case of a measure supported on an interval).

2. Preliminaries

The complex plane is denoted by $\mathbb{C}$, the Riemann sphere by $\hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$, the real line by $\mathbb{R}$ and the extended real line by $\hat{\mathbb{R}} = \mathbb{R} \cup \{\infty\}$.

By a measure μ we will mean a positive bounded Borel measure whose support $\mathrm{supp}(\mu) \subset \hat{\mathbb{R}}$ is an infinite set and normalised such that $\mu(\hat{\mathbb{R}}) = 1$. The inner product in the metric space $L_2(\mu)$ is then defined as

$$\langle f, g \rangle = \int f \bar{g}\, \mathrm{d}\mu. \tag{1}$$

Next, we will introduce the spaces of rational functions with real poles. Let a sequence $A = \{\alpha_1, \alpha_2, \ldots\} \subset \hat{\mathbb{R}} \setminus \{0\}$ be given such that $A \cap \mathrm{supp}(\mu) = \emptyset$. As a consequence we cannot have $\mathrm{supp}(\mu) = \hat{\mathbb{R}}$. Define factors

$$Z_n(z) = \frac{z}{1 - z/\alpha_n}$$

and basis functions

$$b_n(z) = b_{n-1}(z) Z_n(z), \quad b_0 = 1.$$

Then the space of rational functions with poles in A is defined as

$$\mathscr{L}_n = \mathrm{span}\{b_0, \ldots, b_n\}.$$

Let $\mathscr{P}_n$ denote the space of polynomials of degree at most n and define

$$\pi_n(z) = \prod_{k=1}^{n} (1 - z/\alpha_k),$$

then we may write equivalently

$$\mathscr{L}_n = \{p_n/\pi_n,\ p_n \in \mathscr{P}_n\}.$$

Orthonormalising the basis $\{b_0,\dots,b_n\}$ with respect to μ we obtain orthogonal rational functions $\{\phi_0,\dots,\phi_n\}$ where we choose the leading coefficient κ_n in the expansion $\phi_n(z)=\kappa_n b_n(z)+\cdots$ to be real. The ϕ_n will be uniquely determined once the sign of κ_n is fixed. We will get back to this later on. The following lemma from [1] will be useful.

Lemma 1. *The orthonormal functions ϕ_n have real coefficients with respect to the basis $\{b_k\}$.*

It follows, in particular, that $\phi_n(z)$ is real for real z and for any inner product $\langle f,\phi_n\rangle$ we may omit the complex conjugate bar in (1).

The Riesz–Herglotz–Nevanlinna kernel $D(t,z)$ for the real line is defined as

$$D(t,z)=-\mathrm{i}\,\frac{1+tz}{t-z}$$

and the Riesz–Herglotz–Nevanlinna transform of the measure μ as

$$\Omega_\mu(z)=\int D(t,z)\,\mathrm{d}\mu(t).$$

As in the polynomial case we introduce functions of the second kind,

$$\psi_n(z)=\int D(t,z)[\phi_n(t)-\phi_n(z)]\,\mathrm{d}\mu(t)$$

for $n\geqslant 1$ and $\psi_0(z)=\mathrm{i}\,z$. From the previous lemma it follows that $\psi_n(z)$ is purely imaginary for real z, i.e., $\psi_n(z)\in\mathrm{i}\hat{\mathbb{R}}$ if $z\in\hat{\mathbb{R}}$.

The orthogonal rational function ϕ_n is called *regular* if its numerator polynomial p_n satisfies $p_n(\alpha_{n-1})\neq 0$. The system $\{\phi_n\}$ is regular if ϕ_n is regular for every n. We now mention the most important theorem for the computation of orthogonal rational functions on the real line, which states that they satisfy a three-term recurrence relation, analogous to the one for the polynomial case. For the proof of the theorem we refer to [1].

Theorem 2. *Put by convention $\alpha_{-1}=\alpha_0=\infty$. Then for $n=1,2,\dots$ the orthonormal rational functions ϕ_n satisfy the following three term recurrence relation if and only if ϕ_n and ϕ_{n-1} are regular:*

$$\phi_n(z)=\left(E_nZ_n(z)+B_n\frac{Z_n(z)}{Z_{n-1}(z)}\right)\phi_{n-1}(z)-\frac{E_n}{E_{n-1}}\frac{Z_n(z)}{Z_{n-2}(z)}\phi_{n-2}(z). \tag{2}$$

The initial conditions are $\phi_{-1}(z)\equiv 0$, $\phi_0(z)\equiv 1$ and the coefficients E_n are nonzero.

Note that in this case the coefficient E_0 is not used and can be arbitrarily chosen. We take it equal to $E_0=1$. This will influence the expression for ψ_{-1} later on. If we take the coefficient E_n to be positive, then the functions ϕ_n will be uniquely determined. This amounts to fixing the sign of κ_n.

If we take all poles outside the convex hull of $\mathrm{supp}(\mu)$, then the system $\{\phi_n\}$ will be regular and thus the recurrence relation will hold for every n. This follows from the fact that in this case the zeros of ϕ_n are inside the convex hull of $\mathrm{supp}(\mu)$. Therefore, if $\mathrm{supp}(\mu)$ is connected then $\{\phi_n\}$ will be regular (because of the assumptions we made on the location of the poles).

As for the functions of the second kind, we have the following theorem from [1, p. 267].

Theorem 3. *Suppose that the system of orthogonal rational functions ϕ_n is regular and let ψ_n be the functions of the second kind associated with them. Then for $n \geqslant 2$ these ψ_n satisfy the same recurrence relation* (2) *as the ϕ_n.*

If we want to start the recursion from $n = 1$ we will need an expression for $\psi_{-1}(z)$, which will be given in the following lemma.

Lemma 4. *In order to satisfy recurrence relation* (2) *for $n = 1$, $\psi_{-1}(z)$ has to be defined as*

$$\psi_{-1}(z) = \mathrm{i}(1 + z^2).$$

Proof. This is a matter of straightforward calculation. Compute ψ_1 using the definition and compare it with the expression obtained using the recurrence relation. □

3. Interpolation properties for Ω_μ

In this section, we will derive certain interpolation properties for the Riesz–Herglotz–Nevanlinna transform $\Omega_\mu(z)$ which will be used to provide an algorithm to compute the recursion coefficients E_n and B_n. It may seem more natural to use the Stieltjes transform instead of the Riesz–Herglotz–Nevanlinna transform, but then the functions of the second kind would have to be defined in a different way as well and we prefer to be consistent with the definitions and notation of [1] and related articles.

First we need a simple lemma.

Lemma 5. *Let $D(t,z)$ be the Riesz–Herglotz–Nevanlinna kernel as defined above and $\phi_n(z)$ the orthonormal rational function. Then for any f such that* (*as a function of t*) $D(t,z)[f(t) - f(z)] \in \mathscr{L}_{n-1}$ *we have*

$$\int D(t,z)\phi_n(t)\,\mathrm{d}\mu(t) = \frac{1}{f(z)} \int D(t,z)\phi_n(t) f(t)\,\mathrm{d}\mu(t).$$

This holds in particular if $f \in \mathscr{L}_{n-1}$.

Proof. It follows from $\phi_n \perp \mathscr{L}_{n-1}$ and the remark following Lemma 1 that

$$\int \phi_n(t) D(t,z)[f(t) - f(z)]\,\mathrm{d}\mu(t) = 0.$$

The result is now immediate. □

With this lemma we can easily prove the following interpolation result for Ω_μ. The same result could also be obtained using interpolating polynomials, as in [1, pp. 328–334], but then the argument is a lot more involved.

Theorem 6. *Let Ω_μ be the Riesz–Herglotz–Nevanlinna transform of the measure μ. Let ϕ_n be the orthonormal functions and ψ_n the associated functions of the second kind. Then we have*

$$\psi_n(z) + \phi_n(z)\Omega_\mu(z) = \frac{R_n(z)}{b_{n-1}(z)}, \quad n \geqslant 1 \tag{3}$$

with $R_n(z)$ defined by

$$R_n(z) = \int D(t,z) b_{n-1}(t)\phi_n(t)\,\mathrm{d}\mu(t)$$

and $R_n(z)$ is finite for $z \in \hat{\mathbb{C}} \setminus \mathrm{supp}(\mu)$. Equivalently,

$$\psi_n(z) + \phi_n(z)\Omega_\mu(z) = -\mathrm{i}\,\frac{1+z^2}{b_{n-1}(z)} \int \frac{\phi_n(t) b_{n-1}(t)}{t-z}\,\mathrm{d}\mu(t). \tag{4}$$

If all poles are outside the convex hull of $\mathrm{supp}(\mu)$ then $-\psi_n/\phi_n$ interpolates Ω_μ in Hermite sense in the points $\{\mathrm{i}, -\mathrm{i}, \alpha_1, \alpha_1, \ldots, \alpha_{n-1}, \alpha_{n-1}, \alpha_n\}$.

Proof. Use the definition of ψ_n and Ω_μ to write

$$\psi_n(z) + \phi_n(z)\Omega_\mu(z) = \int D(t,z)\phi_n(t)\,\mathrm{d}\mu(t). \tag{5}$$

The first result then follows from Lemma 5 with $f = b_{n-1}$. To obtain the second equation, write

$$D(t,z) = -\mathrm{i}\left(z + \frac{1+z^2}{t-z}\right)$$

and use the orthogonality of ϕ_n. This yields (4). Dividing by $\phi_n(z)$ we obtain

$$\frac{\psi_n(z)}{\phi_n(z)} + \Omega_\mu(z) = -\mathrm{i}(1+z^2)\frac{\pi_{n-1}(z)}{z^{n-1}}\,\frac{\pi_n(z)}{p_n(z)} \int \frac{\phi_n(t) b_{n-1}(t)}{(t-z)}\,\mathrm{d}\mu(t),$$

where p_n is the numerator of ϕ_n. If all poles are outside the convex hull of $\mathrm{supp}(\mu)$, then none of the zeros of p_n will coincide with any of the poles, hence the Hermite interpolation. $\square$

It follows from (5) that $\psi_n(z) + \phi_n(z)\Omega_\mu(z)$ is the nth Fourier coefficient of $D(t,z)$ as a function of t, relative to the orthonormal system $\{\phi_k\}$. Therefore,

$$\lim_{n\to\infty} \frac{R_n(z)}{b_{n-1}(z)} = 0, \quad z \in \hat{\mathbb{C}} \setminus \mathrm{supp}(\mu). \tag{6}$$

This is an easy consequence of Bessel's inequality, see e.g., [8, p. 85]. Without further assumptions on the measure nothing can be said for $z \in \mathrm{supp}(\mu)$, since $D(t,z)$ may not be in $L_2(\mu)$.

4. An algorithm to compute E_n and B_n

In the rest of this paper we assume that the system $\{\phi_n\}$ is regular. Then since both ϕ_n and ψ_n satisfy recurrence relation (2), so does $\psi_n + \phi_n \Omega_\mu$. Therefore, we have from (3) for $n \geqslant 3$,

$$\frac{R_n}{b_{n-1}Z_n} = (E_n Z_{n-1} + B_n)\frac{R_{n-1}}{b_{n-2}Z_{n-1}} - \frac{E_n}{E_{n-1}}\,\frac{R_{n-2}}{b_{n-3}Z_{n-2}}.$$

We formally define $R_{-1}(z)$ and $R_0(z)$ using (3) so that the recursion also holds for $n = 1, 2$ as follows

$$R_{-1}(z) = \mathrm{i}(1+z^2), \quad R_0(z) = \mathrm{i}\,z + \Omega_\mu(z). \tag{7}$$

Putting

$$\Gamma_n(z) = \frac{b_{n-2}(z)}{b_{n-1}(z)}\,\frac{Z_{n-1}(z)}{Z_n(z)}\,\frac{R_n(z)}{R_{n-1}(z)}, \quad n \geqslant 0 \tag{8}$$

where $b_k(z) \equiv 1$ if $k \leqslant 0$, we get the following recurrence relation

$$\Gamma_n(z) = E_n Z_{n-1}(z) + B_n - \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)}, \quad n \geqslant 1. \tag{9}$$

Note that for $n \geqslant 2$ the expression for Γ_n reduces to

$$\Gamma_n(z) = \frac{1 - z/\alpha_n}{z}\,\frac{R_n(z)}{R_{n-1}(z)}, \quad n \geqslant 2$$

and for $n = 1$ we have

$$\Gamma_1(z) = (1 - z/\alpha_1)\frac{R_1(z)}{R_0(z)}.$$

Since $R_n(z)$ is finite for any z outside $\mathrm{supp}(\mu)$ and because none of the poles is in $\mathrm{supp}(\mu)$, it follows that $\Gamma_n(\alpha_n) = 0$ for $n \geqslant 1$. The initial condition for the recurrence relation follows from (7) and (8),

$$\Gamma_0(z) = \frac{\mathrm{i}z + \Omega_\mu(z)}{\mathrm{i}(1+z^2)}.$$

With the definition of Ω_μ this can be rewritten as

$$\Gamma_0(z) = -\int \frac{\mathrm{d}\mu(t)}{t - z}. \tag{10}$$

It follows that $-\Gamma_0(z)$ is the Stieltjes transform of the measure μ, see, e.g., [6].

The functions $\Gamma_n(z)$ are closely related to certain functions arising in a modified Schur algorithm, as described in [7]. For the case of cyclicly repeated poles $\{\alpha_1, \ldots, \alpha_p, \alpha_1, \ldots, \alpha_p, \ldots\}$, the author defines Nevanlinna functions $F_n(z)$ which after careful consideration turn out to be equal to the Γ_n functions (up to a multiplicative constant only depending on n). For more information we refer to his article.

Eq. (9) obviously gives rise to a continued fraction expansion for the function $-\Gamma_0(z)$. The approximants of this continued fraction are multipoint Padé approximants for the Stieltjes transform of μ. A detailed description can be found in [2].

Using recursion formula (9) it is possible to compute the recursion coefficients E_n and B_n in (2). In the rest of this section we assume that all poles are different from each other. We will get back to this at the end of the section. Using the fact that $\Gamma_n(\alpha_n)=0$ we easily find that

$$B_n = -E_n Z_{n-1}(\alpha_n) + \frac{E_n/E_{n-1}}{\Gamma_{n-1}(\alpha_n)}, \quad n \geqslant 1.$$

To find an expression for E_n we multiply (9) by $\Gamma_{n-1}(z)$ and take the limit for $z \to \alpha_{n-1}$, which gives, using l'Hôpital's rule (and increasing the index $n-1$ to n in the final result)

$$E_n = \frac{-1}{\alpha_n^2 \Gamma_n'(\alpha_n)}.$$

This is of course not a very useful expression, because it still involves (the derivative of) Γ_n to compute E_n. Differentiating (9) however gives

$$\Gamma_n'(z)/E_n = Z_{n-1}'(z) + \frac{\Gamma_{n-1}'(z)/E_{n-1}}{\Gamma_{n-1}^2(z)}$$

or defining $\Delta_n(z) = \Gamma_n'(z)/E_n$ we may write

$$\Delta_n(z) = Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)}{\Gamma_{n-1}^2(z)}, \quad n \geqslant 1 \tag{11}$$

and $\Delta_0(z) = \Gamma_0'(z)$. We finally substitute this into the expression for E_n to find

$$E_n = \frac{1}{|\alpha_n|}\sqrt{\frac{-1}{\Delta_n(\alpha_n)}}, \quad n \geqslant 1.$$

This concludes our discussion. To compute E_n and B_n we will need Γ_0 and its derivative in the poles $\{\alpha_1, \ldots, \alpha_n\}$.

In the case of repeated poles, we will need higher-order derivatives of $\Gamma_0(z)$. Consider for example the case where for a certain value of n we would have $\alpha_n = \alpha_{n-1}$. To compute B_n we cannot simply substitute α_n for z in (9) since α_n is also a zero of $Z_{n-1}(z)$ and $\Gamma_{n-1}(z)$. This is only another formulation of [1, Theorem 11.10.3], which states that for a pole α with multiplicity $\alpha^{\#}$ you need the first $2\alpha^{\#}-1$ derivatives of Ω_μ (and thus of Γ_0) to characterise the inner product. Indeed if all poles are different from each other, we only need Γ_0 and its derivative.

5. Examples

Before we go into a numerical analysis of the error propagation in the algorithm derived in the previous section, we look at some examples. In all examples, $\mathrm{supp}(\mu)$ is connected and the poles are simple, so we can use the algorithm to compute the recursion coefficients.

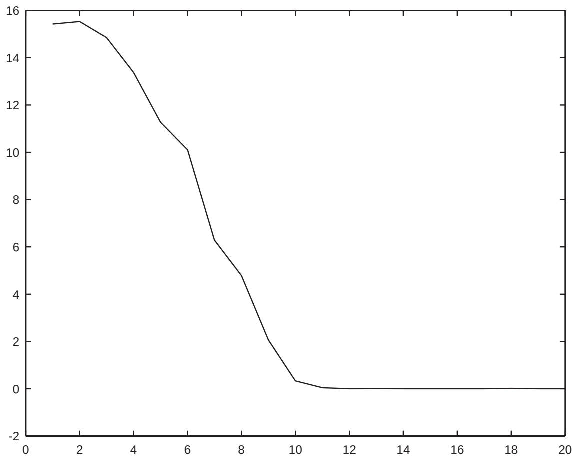

Fig. 1. Number of correct digits of E_n against n, example 1.

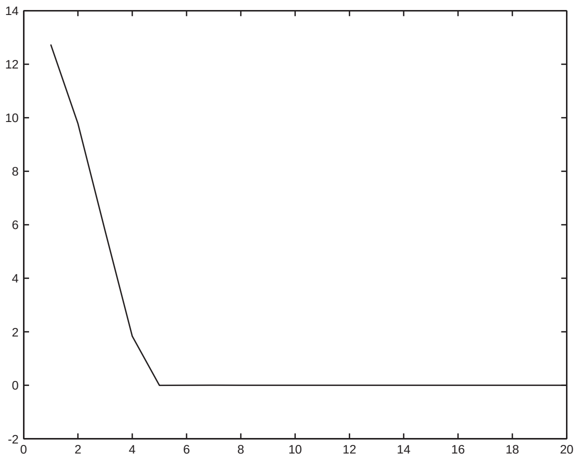

Fig. 2. Number of correct digits of E_n against n, example 2.

First, consider the sequence of poles $\{\omega, -\omega, 2\omega, -2\omega, \ldots\}$ where $\omega = 1.1$. We use the normalised Lebesgue measure on the interval $[-1, 1]$, so we have $\mathrm{d}\mu(z) = 1/2\mathrm{d}z$. For this case some computations yield

$$\Gamma_0(z) = \frac{1}{2} \ln \frac{z+1}{z-1}, \quad z \in \hat{\mathbb{C}} \setminus [-1, 1].$$

In Fig. 1 the number of correct digits in double precision for the coefficient E_n is plotted against n. All computations were done in Maple, using 16 digits for double precision and 80 for the "exact" values. It seems that for $n = 10$ we have already lost *all* correct digits.

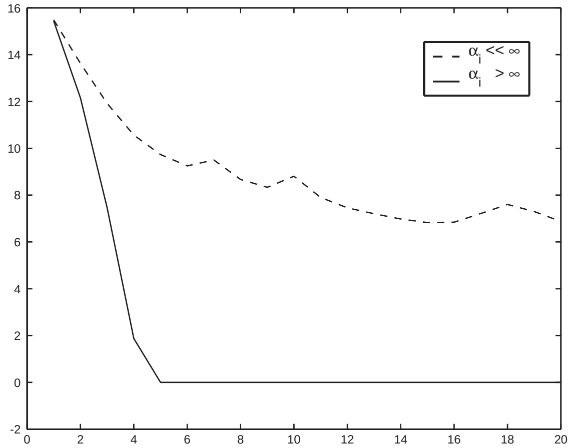

Fig. 3. Number of correct digits of E_n against n, poles tending to infinity (solid line) and poles tending to zero (dashed line).

In the next example the poles are at $\alpha_i = -10 + 5/i,\ i = 1, 2, \ldots$ and the weight function is e^{-z} on the half-line $[0, \infty)$. In this case we have

$$\Gamma_0(z) = \mathrm{Ei}(z)e^{-z}, \quad z \in \hat{\mathbb{C}} \setminus [0, \infty),$$

where $\mathrm{Ei}(z)$ is the analytic continuation of the exponential integral, defined for real $z < 0$ as $\int_{-\infty}^{z} e^t/t\,\mathrm{d}t$. Again we plotted the number of correct digits for E_n against n (Fig. 2). Here the situation is even worse than in the previous example. We have lost all correct digits for $n = 5$.

Next, we wish to look at how the location of the poles influences the computations. In Fig. 3 we compare the number of correct digits for different poles. As in the last example we have the weight function e^{-z} on the half-line $[0, \infty)$. In solid line is the number of correct digits for poles located at $\alpha_i = -10^{i-1},\ i = 1, 2, \ldots$ and tending to infinity very fast, while for the dashed line the poles are at $\alpha_i = -1/2^{i-1},\ i = 1, 2, \ldots$ and tend to zero. In this case we still have six correct digits for $n = 20$, while for the poles tending to infinity we have lost all digits for $n = 5$.

6. Properties of Δ_n

The following theorem can be found in [1, Chapter 11, Section 3].

Theorem 7. *Let ϕ_n be the orthonormal functions and let ψ_n be the functions of the second kind. Define*

$$\chi_n(z; s) = \psi_n + s\phi_n(z).$$

Then for arbitrary complex s and t,

$$\frac{\chi_n(w;t)\chi_{n-1}(z;s)}{Z_n(w)Z_{n-1}(z)} - \frac{\chi_n(z;s)\chi_{n-1}(w;t)}{Z_n(z)Z_{n-1}(w)}$$
$$= -\frac{z-w}{zw} E_n \left[\sum_{k=1}^{n-1} \chi_k(z;s)\chi_k(w;t) + [st - 1 + D(z,w)(t-s) \right]$$

with E_n the recursion coefficient and $D(z,w)$ the Riesz–Herglotz–Nevanlinna kernel.

With the aid of this theorem we are able to prove that the functions $\Delta_n(z)$ are nonpositive for real z outside $\operatorname{supp}(\mu)$.

Theorem 8. *With $\Delta_n(z)$ as defined above we have*

$$\Delta_n(z) \leqslant 0, \quad z \in \mathbb{R} \setminus \operatorname{supp}(\mu).$$

The inequality is strict for $z \notin \{\alpha_1, \alpha_2, \ldots, \alpha_{n-1}\}$.

Proof. First, note that for real z the functions χ_n, Ω_μ and Ω'_μ are purely imaginary, so we may write for example $|\Omega_\mu(z)|^2 = -(\Omega_\mu(z))^2$.

It follows from the definition of $\Gamma_n(z)$ that

$$\Gamma_n(z) = \frac{\chi_n(z)}{Z_n(z)} \Big/ \frac{\chi_{n-1}(z)}{Z_{n-1}(z)},$$

where $\chi_n(z) = \psi_n(z) + \phi_n(z)\Omega_\mu(z)$. Taking derivatives and dividing by E_n we obtain

$$\Delta_n(z) = \frac{1}{E_n} \left[\left(\frac{\chi_n(z)}{Z_n(z)} \right)' \frac{\chi_{n-1}(z)}{Z_{n-1}(z)} - \frac{\chi_n(z)}{Z_n(z)} \left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)} \right)' \right] \Big/ \left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)} \right)^2.$$

Now use Theorem 7 with $s = \Omega_\mu(z)$ and $t = \Omega_\mu(w)$, where z and w are in $\mathbb{R} \setminus \operatorname{supp}(\mu)$. If we divide by $(z-w)$ and let w tend to z, some calculations yield

$$\frac{1}{E_n} \left[\left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)} \right)' \frac{\chi_n(z)}{Z_n(z)} - \frac{\chi_{n-1}(z)}{Z_{n-1}(z)} \left(\frac{\chi_n(z)}{Z_n(z)} \right)' \right]$$
$$= -\frac{1}{z^2} \left[\sum_{k=1}^{n-1} \chi_k^2(z) + \Omega_\mu^2(z) - 1 + \mathrm{i}(1+z^2)\Omega'_\mu(z) \right],$$

which, using the definition of Ω_μ and the fact that $z \in \mathbb{R}$, may be written

$$\frac{1}{E_n} \left[\left(\frac{\chi_n(z)}{Z_n(z)} \right)' \frac{\chi_{n-1}(z)}{Z_{n-1}(z)} - \frac{\chi_n(z)}{Z_n(z)} \left(\frac{\chi_{n-1}(z)}{Z_{n-1}(z)} \right)' \right]$$
$$= -\frac{1}{z^2} \left[\sum_{k=1}^{n-1} |\chi_k(z)|^2 + |\Omega_\mu(z)|^2 + 1 - (1+z^2)|\Omega'_\mu(z)| \right].$$

Recall that $\chi_n(z)$ is the nth Fourier coefficient of $D(t,z)$ as a function of t, relative to the orthonormal system $\{\phi_k\}$ and note that we have

$$1-(1+z^2)|\Omega'_\mu(z)| = -\int |D(t,z)|^2\,\mathrm{d}\mu(t).$$

This is a matter of straightforward computation.

Putting all the previous results together we have the following expression for the function $\Delta_n(z)$ when $z \in \mathbb{R}\setminus \mathrm{supp}(\mu)$,

$$\Delta_n(z) = \frac{1}{z^2}\left|\frac{Z_{n-1}(z)}{\chi_{n-1}(z)}\right|^2 \left[\sum_{k=0}^{n-1}\left|\int D(t,z)\phi_k(t)\,\mathrm{d}\mu(t)\right|^2 - \int |D(t,z)|^2\,\mathrm{d}\mu(t)\right]. \tag{12}$$

It follows from Bessel's inequality that

$$\sum_{k=0}^{n-1}\left|\int D(t,z)\phi_k(t)\,\mathrm{d}\mu(t)\right|^2 \leqslant \int |D(t,z)|^2\,\mathrm{d}\mu(t)$$

with equality only when $D(t,z)$ (as a function of t) is an element of $\mathscr{L}_{n-1}$. This happens only for $z\in\{\alpha_1,\alpha_2,\ldots,\alpha_{n-1}\}$. Note that $\int D(t,z)\phi_k(t)\,\mathrm{d}\mu(t) = R_k(z)/b_{k-1}(z)$ and that $Z_{n-1}(z)b_{n-2}(z) = b_{n-1}(z)$. Using this and again Bessel's inequality we may write

$$\Delta_n(z) \leqslant -\frac{1}{z^2}\left|\frac{b_{n-1}(z)}{R_{n-1}(z)}\right|^2 \sum_{k=n}^{\infty}\left|\frac{R_k(z)}{b_{k-1}(z)}\right|^2 \leqslant 0.$$

The first inequality becomes an equality if the system $\{\phi_k\}$ is dense in $L_2(\mu)$ (this is [8, Theorem 4.18]) and the second inequality is an equality for $z=\alpha_k$, $1\leqslant k\leqslant n-1$ only when α_k is a zero of $R_m(z)$ for every $m\geqslant n$ and is not a zero of $R_{n-1}(z)$. This proves the theorem. □

From the proof of this theorem we have the following corollary.

Corollary 9. *Assume that* $\mathrm{supp}(\mu)$ *is bounded from at least one side. Then it follows that*

$$\lim_{z\to\infty} \Delta_n(z) = 0$$

with z tending to infinity in the unbounded component of $\hat{\mathbb{R}}\setminus\mathrm{supp}(\mu)$.

Proof. The proof is immediate from formula (12) and the definition of $D(t,z)$. □

7. Error analysis

Let us assume that we know all the coefficients E_k and B_k exactly for $k=1,\ldots,n$ and we wish to compute E_{n+1} and B_{n+1}. The only errors in this case would be initial errors on our data (Γ_n and Δ_n evaluated in the poles) that become large with increasing n through formula (9). If we denote the computed Γ_n-function by $\tilde{\Gamma}_n(z)$ then the relative error $\gamma_n^r(z)$ equals $(\tilde{\Gamma}_n(z)-\Gamma_n(z))/\Gamma_n(z)$. Furthermore, we also assume that the error on $Z_n(z)$ is negligible compared to $\gamma_n^r(z)$. From the recurrence relation for $\Gamma_n(z)$ we find

$$\begin{aligned}\tilde{\Gamma}_n(z) &= E_n Z_{n-1}(z) + B_n - \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)(1+\gamma_{n-1}^r(z))}\\ &\approx E_n Z_{n-1}(z) + B_n - \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)}(1-\gamma_{n-1}^r(z))\\ &\approx \Gamma_n(z) + \frac{E_n/E_{n-1}}{\Gamma_{n-1}(z)}\gamma_{n-1}^r(z),\end{aligned}$$

so we find for the relative error $\gamma_n^r(z)$ that

$$\gamma_n^r(z) \approx \frac{E_n/E_{n-1}}{\Gamma_n(z)\Gamma_{n-1}(z)}\,\gamma_{n-1}^r(z).$$

Writing this recursion explicitly and using the defining relation (8) we obtain after some calculations

$$\gamma_n^r(z) \approx \mathrm{i}\,\frac{E_n b_n(z) b_{n-1}(z)(1+1/z^2)R_0(z)}{R_n(z)R_{n-1}(z)}\,\gamma_0^r(z)$$

and if we assume that the errors $\gamma_0^r(z)$ on the data are bounded by the machine precision ε, then we obtain the following bound:

$$|\gamma_n^r(z)| \leqslant \left|\frac{E_n b_n(z) b_{n-1}(z)(1+1/z^2)R_0(z)}{R_n(z)R_{n-1}(z)}\right|\varepsilon$$

or using the definition of b_n,

$$|\gamma_n^r(z)| \leqslant \left|\frac{R_n(z)}{b_{n-1}(z)}\,\frac{R_{n-1}(z)}{b_{n-2}(z)}\left(\frac{1}{z}-\frac{1}{\alpha_n}\right)\left(\frac{1}{z}-\frac{1}{\alpha_{n-1}}\right)\frac{1}{E_n R_0(z)(1+1/z^2)}\right|^{-1}\varepsilon.$$

To compute B_n we need the function $\Gamma_{n-1}(z)$ evaluated in the pole α_n. It follows from Eq. (6) that the error will become unbounded as long as α_n and E_n do not tend to zero. This may explain why in Fig. 3 we obtain better results for the poles tending to zero. The asymptotic behaviour of E_n obviously depends on the measure μ and the location of the poles. For a measure supported on the interval $[-1,1]$ and satisfying the condition $\mu' > 0$ a.e. (where μ' is the Radon–Nikodym derivative of the measure μ with respect to the Lebesgue measure), we can use the results from [3]. It follows that E_n is bounded away from zero if the poles are bounded away from the interval. Using the conformal mapping

$$\tau(z) = \frac{1-z}{1+z}, \quad z \in [-1,1],$$

we can obtain similar results for measures supported on the half-line $[0,\infty)$. In this case, the error will become unbounded if the poles stay away from infinity and from zero. This explains the behaviour of the first two examples in Section 5.

Next, we will look at the relative error $\delta_n^r(z)$ on $\Delta_n(z)$. We assume that the error on $Z_n'(z)$ is negligible compared to $\delta_n^r(z)$. From (11) we obtain

$$\begin{aligned}\tilde{\Delta}_n(z) &= Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)(1+\delta_{n-1}^r(z))}{(\Gamma_{n-1}(z)(1+\gamma_{n-1}^r(z)))^2} \\ &\approx Z_{n-1}'(z) + \frac{\Delta_{n-1}(z)}{\Gamma_{n-1}^2(z)}(1+\delta_{n-1}^r(z) - 2\gamma_{n-1}^r(z)) \\ &\approx \Delta_n(z) + (\Delta_n(z) - Z_{n-1}'(z))(\delta_{n-1}^r(z) - 2\gamma_{n-1}^r(z)).\end{aligned}$$

The relative error $\delta_n^r(z)$ thus equals

$$\delta_n^r(z) \approx \left(1 - \frac{Z_{n-1}'(z)}{\Delta_n(z)}\right)(\delta_{n-1}^r(z) - 2\gamma_{n-1}^r(z))$$

and a bound is given by

$$|\delta_n^r(z)| \leqslant \left|1 - \frac{Z_{n-1}'(z)}{\Delta_n(z)}\right|(|\delta_{n-1}^r(z)| + 2|\gamma_{n-1}^r(z)|). \tag{13}$$

It is difficult to write this error bound in an explicit form like the one for γ_n^r. To compute the coefficient E_n we need $\Delta_n(\alpha_n)$. For the poles tending to infinity in Fig. 3, we can use Corollary 9 and formula (13) to explain why the error becomes unbounded.

8. Conclusion

The algorithm presented here, although simple and easily implemented, is not very useful in practical applications (working in double precision) because of the unbounded error growth. It is, however, a useful tool for research purposes where efficiency and speed are not an issue and one can use multiprecision arithmetic. It works for any measure satisfying the conditions of Section 2 and simple poles outside the convex hull of this measure. In [4] we will present a more useful algorithm to compute the recurrence coefficients, based on explicit formulas involving inner products and derive accurately computable error bounds for these formulas. This will provide an algorithm which can be used in practical applications.

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